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Title: Design of State-of-the-art Flow Cells for Energy Applications

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## Design of State-of-the-art Flow Cells for Energy Applications

**Motivation:** The worldwide energy demand is increasing every day and it necessitates rational and efficient usage of renewable energy. Undoubtedly, utilization of renewable energy can address various environmental challenges. However, all current renewable energy resources (wind, solar, and hydroelectric power) are intermittent and fluctuating in their nature that raises an important question of introducing effective energy storage solutions. Utilization of redox flow cells (RFCs) has recently been recognized as a viable technology for large-scale energy storage and, hence, is well suited for integrating renewable energy and balancing electricity grids. In brief, RFC is an electrochemical storage device (Fig. 1), where energy is stored in chemical bonds, similar to a battery, but with reactants external to the cell. The state-of-the-art in flow cell technology uses an aqueous acidic electrolyte and simple metal redox couples. Several of these systems have been commercialized although current technologies, such as vanadium (V) and zinc-bromine ($Zn$-$Br_2$) RFCs, for grid level energy storage, suffer from a number of drawbacks, i.e. expensive and resource-limited active materials (vanadium RFCc), and low current performance ($Zn$-$Br_2$ RFCs due to Zn dendrite formation). Thus, *there is an urgent call to develop efficient (high-energy density) and low-cost RFCs to meet the efflorescent energy storage demands*.

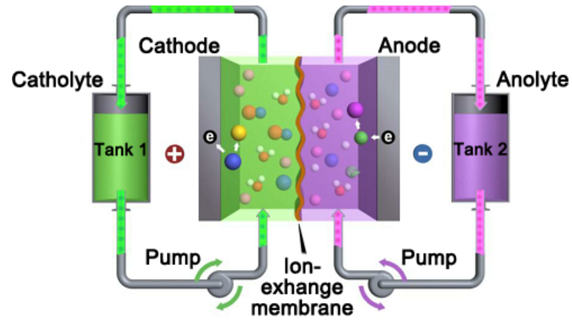


**Fig. 1**. A schematic diagram of a redox flow cell

**Approach:** To address the first challenge of achieving high-energy density, we plan to design and further modify complexes composed of bifunctional multidentate ligands and specific metal centers, capable of storing as many electrons as possible. This can be achieved by using one metal center, which can possess multiple oxidation states, and/or by introducing multi metal centers. To accommodate more electrons, we plan to adapt ligands accordingly (change the bite angle of the ligand and add/remove electron-withdrawing or electron-donating groups to the adjustable group (R) or changing its size) to enhance stability of these complexes and tune their redox potentials (Fig. 2). In order to address the second challenge of reducing cost of the RFCs, we plan to use iron (Fe) metal as it regularly occupies multiple oxidation states and is the second most abundant metal in the earth's crust that makes it an ideal metal for improved energy densities, higher potentials, and numbers of electrons per molecule while maintaining potential cost competitiveness. This will provide us with a vast range of possibilities to explore various binding sites of Fe in relation to its oxidation states. Theoretical modeling of ionic liquids (IL) and solute-IL systems is an essential component of this project, providing electronic structure information that will help predict redox behavior of complexes of interest. Density functional theory calculations considering solvation effects will be performed to yield accurate predictions of redox potentials. Critical for these studies will be the appropriate inclusion of multireference states and the investigation of electron localization and delocalization patterns at the metal center and ligands.

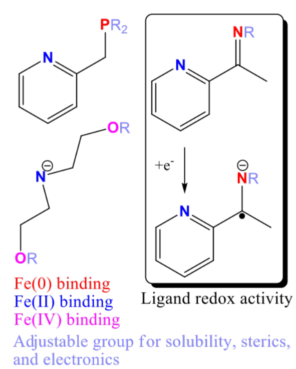


**Fig. 2**. Examples of tunable complexes

**Impact:** The scientific results of the project will not only spark further experimental verification of the proposed RFCs (by Mukund at MPA), but will also be used as a general guideline towards the realization of novel inexpensive, safe, and high-performance flow cells, which could be implemented in the electricity grids in the near future. This project directly responds to the aim of approaching DOE's cost target on large-scale energy storage, \$150/kWh, and LANL's Strategic Investment Plan on Energy Storage. Having developed such systems, people will be able to effectively store and use greener electricity rather than relying on carbon energy sources, such as fossil fuels, which the world will run out sooner or later.

I confirm that I wrote this proposal and will perform this research during my postdoctoral appointment.

Ivan A. Popov